2-(Methylsulfanyl)quinoxaline
21948-73-2 | DTXSID00325902

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.08e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.33e-01

Confidence level: 3.60e-01

Nearest Neighbors from the Training Set

Image not found

Dazomet
Measured: 1.85e-02
Predicted: 2.18e-02

Image not found

Bis(ethylxanthogen)
Measured: 1.14e-05
Predicted: 4.06e-05

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2,5-Cyclohexadien-1-one, 2,6-dibromo-4-(chloroimino)-
Measured: 1.96e-04
Predicted: 1.41e-03

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Chloranil
Measured: 1.02e-03
Predicted: 3.29e-03